

Semiclassical quantization by Padé approximant to periodic orbit sums

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Abstract. – Periodic orbit quantization requires an analytic continuation of non-convergent semiclassical trace formulae. We propose a method for semiclassical quantization based upon the Padé approximant to the periodic orbit sums. The Padé approximant allows the re-summation of the typically exponentially divergent periodic orbit terms. The technique does not depend on the existence of a symbolic dynamics and can be applied to both bound and open systems. Numerical results are presented for two different systems with chaotic and regular classical dynamics, viz. the three-disk scattering system and the circle billiard.

Semiclassical theories link the spectrum of a quantum system to the dynamics of its classical counterpart and thereby play an important rôle in the deeper understanding of the relation between quantum and classical mechanics. Of particular interest are periodic orbit theories which describe the quantum mechanical density of states in terms of contributions from the periodic orbits of the classical system. The semiclassical trace formulae have been derived by Gutzwiller for classically chaotic systems [1, 2] and by Berry and Tabor for regular (integrable) systems [3]. A common feature of these formulae is that in most cases the periodic orbit sum does not converge in those regions where the semiclassical eigenenergies or resonances are located. These resonances are given as the poles of the periodic orbit sum,

$$g(E) = \sum_{\text{po}} \mathcal{A}_{\text{po}}(E) e^{i[S_{\text{po}}(E)/\hbar - \frac{\pi}{2}\mu_{\text{po}}]} , \quad (1)$$

where \mathcal{A}_{po} , S_{po} , and μ_{po} are the amplitude, classical action and Maslov index of the periodic orbit (po), respectively. Formulae for the amplitudes \mathcal{A}_{po} are given in refs. [2, 3].

In the last decade various techniques have been developed to circumvent the convergence problem of periodic orbit theory. Examples are the cycle expansion technique [4, 5, 6, 7], the Riemann-Siegel type formula and pseudo-orbit expansions [8], and a periodic orbit quantization rule for the counting function of eigenvalues [9]. These techniques have been proven to be very

efficient for systems with special properties, *e.g.*, the cycle expansion for hyperbolic systems with an existing symbolic dynamics, and the other methods for the calculation of bound spectra. Recently, a method for periodic orbit quantization has been introduced [10, 11, 12] which is based on the high resolution analysis (harmonic inversion) of the semiclassical recurrence signal. The method requires the knowledge of the periodic orbits up to a given maximum period (classical action), which depends on the mean density of states (*i.e.*, the Heisenberg time), and can be applied to open or bound systems with regular, chaotic, or even mixed [13] classical dynamics.

In this Letter we propose an alternative method for periodic orbit quantization. It is the Padé approximant (PA) to slowly convergent and/or divergent periodic orbit sums. In the former or the latter case, the PA either significantly increases the convergence rate or analytically continues the *exponentially* divergent series. The PA is especially robust for re-summing diverging series in many applications in mathematics and theoretical physics [14]. An important example is the summation of the divergent Rayleigh-Schrödinger quantum mechanical perturbation series for, *e.g.*, atoms in electric [15] and magnetic [16] fields. In periodic orbit theory the PA has been applied to cycle-expanded Euler products and dynamical zeta functions [5]. However, to the best of our knowledge, the PA has not yet been used for the direct summation of periodic orbit terms.

Padé approximant (PA) to the periodic orbit sums. – The PA to a complex function $f(z)$ is defined as a ratio of two polynomials and can be computed from the coefficients a_n of the Maclaurin expansion of $f(z)$, *i.e.*, a power series $f(z) = \sum_{n=0}^{\infty} a_n z^n$ with finite or even zero radius of convergence in z [16]. However, eq. (1) does not have the functional form of a Maclaurin power series expansion of $g(E)$ in the energy E . Even disregarding this limitation, a direct computation of the PA to the sum in eq. (1) would be numerically unstable due to the typically large number of periodic orbit terms. Nevertheless, considering E as a parameter, $g(E)$ can be rearranged and written as a formal power series in an auxiliary variable z ,

$$g(z; E) = \sum_n (-iz)^n \left[\sum_{\mu_{\text{po}}=n} \mathcal{A}_{\text{po}}(E) e^{iS_{\text{po}}(E)/\hbar} \right] \equiv \sum_n a_n(E) z^n , \quad (2)$$

where the maximal value of n required for convergence of the PA is relatively small compared with the number of periodic orbit terms. Of course, the arrangement (2) of the periodic orbit sum as a power series is not unique, and expansions similar to eq. (2) can be used for other ordering parameters n of the orbits, *e.g.*, the cycle length in systems with an existing symbolic code. However, if no symbolic dynamics exists, the sorting of orbits by their Maslov index is natural both physically and as a way to introduce an integer summation index and will be justified below by the successful numerical application of the method to a regular system without symbolic dynamics. (For a discussion of the ordering of orbits in cycle-expansion techniques see [17].) Note that the PA to the periodic orbit sum cannot be applied without any ordering parameter, *i.e.*, when no symbolic dynamics exists and all Maslov indices are zero, which is the case, *e.g.*, for the Riemann zeta function as a mathematical model for periodic orbit quantization [11]. The true value $g(E)$ of the periodic orbit sum is obtained by setting $z = 1$ in eq. (2), *i.e.*, $g(E) = g(1; E)$. In such a case, we have a point PA which is given as a ratio of two polynomials in z whose coefficients are non-polynomial functions of E all at a fixed value of z . The usual implementation of the PA as a ratio of two polynomials in z whose coefficients are computed, *e.g.*, via the Longman algorithm [18] would be advantageous if $g(z; E)$ were required for many values of z . In the present case, at each given energy E only one fixed value $z = 1$ is needed and the PA is most efficiently computed by means of the recursive Wynn ε -algorithm [19].

To briefly describe the ε -algorithm, we introduce a sequence of partial sums $\{A_n\}$ which converges to (or diverges from) its limit A as $n \rightarrow \infty$. In the case of divergence, A is called the ‘anti-limit’ of $\{A_n\}$, as $n \rightarrow \infty$. Further, let F be a transformation which maps $\{A_n\}$ into another sequence $\{B_n\}$. The mapping F will represent an accelerator, *i.e.*, sequence $\{B_n\}$ will converge to the same limit A faster than $\{A_n\}$ if the following condition is fulfilled: $(B_n - B)/(A_n - A) \rightarrow 0$, as $n \rightarrow \infty$. In addition, the same F can be applied to wildly divergent sequences $\{A_n\}$. Only non-linear mappings can simultaneously accomplish both goals to accelerate slowly convergent and induce convergence into divergent sequences. The transformation F will be non-linear if its coefficients depend on A_n , *e.g.*, the so-called e -algorithm of Shanks [20], whose mapping F is the operator e_k which converts sequence $\{A_n\}$ into $\{B_n\}$ via $e_k(A_n) = B_{k,n} = [n + k/k]$ ($n \geq 0$, $n \geq k$). This is the well-known Aitken Δ^2 -iteration process (*i.e.*, the simplest PA, [1/1]) extended to higher orders k . The general term in the k th-order transform $B_{k,n}$ of A_n can be computed efficiently from the stable and recursive ε -algorithm of Wynn [19], *i.e.*, $e_s(A_m) = \varepsilon_{2s}^{(m)} = [m + s/s]$, where

$$\varepsilon_{s+1}^{(m)} = \varepsilon_{s-1}^{(m+1)} + 1/\left(\varepsilon_s^{(m+1)} - \varepsilon_s^{(m)}\right); \quad m, s \geq 0 \quad (3)$$

with $\varepsilon_{-1}^{(m)} = 0$, $\varepsilon_0^{(m)} = A_m$, $\varepsilon_{2s+1}^{(m)} = 1/e_s(\Delta A_m)$ and where Δ is the forward difference operator: $\Delta x_j = x_{j+1} - x_j$. When $\{A_n\}$ is the sequence of partial sums of a power series, the two-dimensional array $\varepsilon_{2s}^{(m-s)}$ yields the upper half of the well known Padé table [m/s]. However, the ε -algorithm need not necessarily be limited to power series.

The procedure to apply the above PA to semiclassical quantization by summation of periodic orbit terms is as follows. For a given system we calculate the periodic orbits up to a chosen maximum ordering parameter $n \leq n_{\max}$ where n can be but is not necessarily related to the Maslov indices of orbits. Note that this set of orbits usually differs from the set of orbits with classical action $S_{\text{po}} \leq S_{\max}$, which is required for periodic orbit quantization by harmonic inversion [10, 11, 12]. From the quantities \mathcal{A}_{po} , S_{po} and μ_{po} of these orbits, we compute the partial sums (*e.g.*, with $n \leq \mu_{\max}$ the Maslov index):

$$A_n = \sum_{\mu_{\text{po}} \leq n} \mathcal{A}_{\text{po}}(E) e^{i[S_{\text{po}}(E)/\hbar - \frac{\pi}{2}\mu_{\text{po}}]}. \quad (4)$$

The sequence $\{A_n\}$ of partial sums is used as input to the ε -algorithm, eq. (3), to obtain a converged value $g(E)$ of the periodic orbit sum (1). The semiclassical eigenenergies or resonances are given as the poles of $g(E)$ and are obtained by searching numerically for the zeroes of the reciprocal function $1/g(E)$. Such a search requires the evaluation of, *e.g.*, $\mathcal{A}_{\text{po}}(E)$ and $S_{\text{po}}(E)$ at complex values of E . This is straightforward for the scaling systems considered in this Letter. The number of the poles of $g(E)$ is not constrained by the size of the sequence $\{A_n\}$ of partial sums since our PA is a ratio of two non-polynomial functions of E . We now demonstrate the power of the method on two physical examples with completely different dynamical properties, viz. the open three-disk billiard and the bound circle billiard.

The three-disk scattering system. – As the first example we consider a billiard system consisting of three identical hard disks with unit radii, $R = 1$, displaced from each other by the same distance d . This simple, albeit non-trivial, scattering system has served as a model for the development of the cycle expansion method [4, 5, 6, 7] and periodic orbit quantization by harmonic inversion [10, 11, 12]. The three-disk scattering system is invariant under the symmetry operations of the group C_{3v} , *i.e.*, three reflections at symmetry lines and two rotations by $2\pi/3$ and $4\pi/3$. Resonances belong to one of the three irreducible subspaces A_1 , A_2 , and E [21]. In the following we concentrate on the resonances of the subspace A_1 . For

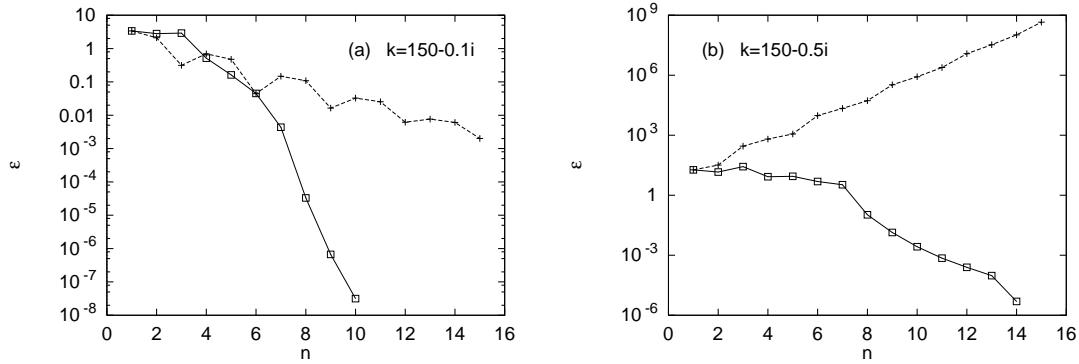


Fig. 1. – Convergence vs. exponential divergence of the partial periodic orbit sums for the three-disk scattering system with $R = 1$, $d = 6$ as functions of the order n at (a) complex wave number $k = 150 - 0.1i$ and (b) $k = 150 - 0.5i$. Dashed lines and plus symbols: Error values $\varepsilon = |A_n - A_{15}^{\text{PA}}|$ for the sequence A_n without Padé approximation. Solid lines and squares: Error values $\varepsilon = |A_n^{\text{PA}} - A_{15}^{\text{PA}}|$ for the Padé approximant A_n^{PA} to the periodic orbit sums.

$d = 6$, semiclassical resonances were calculated by the cycle expansion technique, including periodic orbits up to cycle length $n = 13$ [6, 7]. In order to demonstrate the power of the PA we first apply it to the previously studied case with $R = 1$, $d = 6$. In billiards, which are scaling systems, the shape of periodic orbits does not depend on the energy E , and the classical action is given by the length L of the orbit ($S_{\text{po}} = \hbar k L_{\text{po}}$), where $k = |\mathbf{k}| = \sqrt{2ME}/\hbar$ is the absolute value of the wave vector to be quantized.

We have calculated all periodic orbits with Maslov index $\mu_{\text{po}} \leq 30$, which corresponds to the set of orbits with cycle length $n \leq 15$. The resulting sequence of the partial sums $\{A_n\}$ of periodic orbit terms (eq. 4) converges for wave numbers k above the borderline $\text{Im } k = -0.121557$ [4] which separates the domain of absolute convergence of the periodic orbit sum from the domain where analytic continuation is necessary, but strongly diverges deep in the complex plane, where the resonance poles are located. This is illustrated in fig. 1 for two different wave numbers k . The dashed line and the plus symbols in fig. 1a show the convergence of the sequence $\{A_n\}$ at $k = 150 - 0.1i$. What is plotted is the error values $\varepsilon = |A_n - A_{15}^{\text{PA}}|$, with A_{15}^{PA} the best known approximation to the true limit of the periodic orbit sum. As can be seen this sequence is slowly convergent, and about three significant digits are obtained at $n = 15$. The convergence can be accelerated using the PA, as is seen by the solid line and squares in fig. 1a showing the error values $\varepsilon = |A_n^{\text{PA}} - A_{15}^{\text{PA}}|$ for the sequence of the Padé approximants $\{A_n^{\text{PA}}\}$ to the periodic orbit sum. The periodic orbit sum has converged to six significant digits already by $n = 9$. The situation is much more dramatic in the deep complex plane ($\text{Im } k < -0.122$), e.g., at $k = 150 - 0.5i$. Here, the sequence of the partial sums $\{A_n\}$ of periodic orbit terms exhibits *exponential* divergence, as can be seen by the dashed line and plus symbols in fig. 1b. Nevertheless, this sequence converges when subjected to the PA implemented through the ε -algorithm (see the solid line and squares in fig. 1b).

The resonances of the three-disk scattering systems have been obtained by a numerical two-dimensional root search in the complex k -plane for the zeroes of the function $1/g(k)$, where $g(k)$ is the PA to the periodic orbit sum. A typical subset of the semiclassical resonances obtained is presented as crosses in fig. 2a. They agree perfectly with results obtained by the cycle expansion method in refs. [6, 7]. For comparison the results of the cycle expansion [22] are presented as squares. The dashed lines in fig. 2a denote the imaginary parts $\text{Im } k = -0.1$

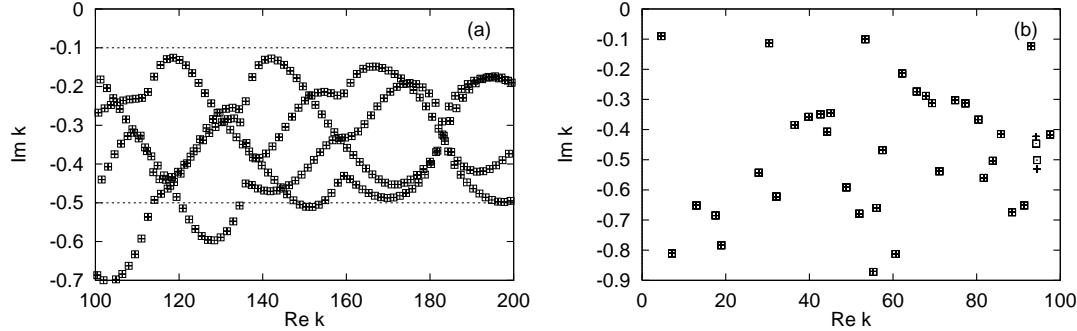


Fig. 2. – (a) Semiclassical resonances (A_1 subspace) for the three-disk scattering system with $R = 1$, $d = 6$. The crosses and squares mark the semiclassical resonances obtained by Padé approximant to the periodic orbit sum and by cycle expansion [22], respectively. The convergence properties of the periodic orbit sum and its Padé approximant are discussed at $\text{Im } k = -0.1$ and $\text{Im } k = -0.5$ marked by the dashed lines (see text). (b) Same as (a) but with small distance $d = 2.5$ between the three disks.

and $\text{Im } k = -0.5$, for which the convergence properties of the periodic orbit sum and the PA has been discussed above.

Calculations similar to those discussed above for $d = 6$ have also been carried out at a shorter distance, $d = 2.5$, between the three disks. The semiclassical resonances obtained by PA to the periodic orbit sum and by cycle expansion [22] are presented as crosses and squares respectively in fig. 2b. Again, the agreement is excellent with the exception of minor discrepancies for the imaginary parts of two resonances with $\text{Re } k \approx 94.3$. It should be noted that the rate of convergence of the PA decreases when the distance d between the disks is reduced as is also the case when cycle-expansion methods are applied. A comparison of the convergence properties of the PA and the cycle-expansion for this specific system will be published elsewhere [23].

The circle billiard. – We now demonstrate the PA to periodic orbit sums for the example of the circle billiard. In sharp contrast to the three-disk system analyzed above, the circle billiard is an integrable and bound system, and, to the best of our knowledge, has not yet been treated by the cycle expansion technique [4] or pseudo-orbit expansion [8]. The exact quantum mechanical eigenvalues $E = \hbar^2 k^2 / 2M$ of the circle billiard are given by zeroes of Bessel functions $J_{|m|}(kR) = 0$, where $m = 0, \pm 1, \pm 2, \dots$ is the angular momentum quantum number and R is the radius of the circle. The semiclassical eigenvalues can be obtained by an Einstein-Brillouin-Keller (EBK) torus quantization [24] resulting in the quantization condition

$$kR\sqrt{1 - (m/kR)^2} - |m|\arccos\frac{|m|}{kR} = \pi\left(n + \frac{3}{4}\right) \quad (5)$$

where $n = 0, 1, 2, \dots$ is the radial quantum number. In the following we choose $R = 1$. The periodic orbits of the circle billiard are those orbits for which the angle between two bounces is a rational multiple of 2π , *i.e.*, the periods L_{po} are obtained from the condition

$$L_{\text{po}} = 2m_r \sin \gamma, \quad (6)$$

with $\gamma \equiv \pi m_\phi / m_r$. Here, $m_\phi = 1, 2, \dots$ is the number of turns of the orbit around the centre of the circle and $m_r = 2m_\phi, 2m_\phi + 1, \dots$ is the number of reflections at the boundary of the circle. Periodic orbits with $m_r \neq 2m_\phi$ can be traversed in two directions and thus have multiplicity

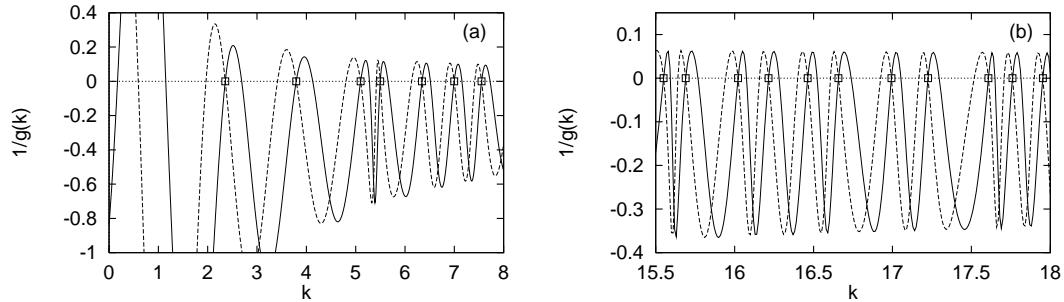


Fig. 3. – Real part (solid line) and imaginary part (dashed line) of the function $1/g(k)$ for the circle billiard with radius $R = 1$ obtained by Padé approximant to the periodic orbit sum. The zeroes agree perfectly with the exact positions of the semiclassical eigenvalues (from eq. 5) marked by the squares.

2. For the amplitudes \mathcal{A}_{po} of the circle billiard, the Berry-Tabor formula [3] for integrable systems yields

$$\mathcal{A}_{\text{po}} = \sqrt{-i\pi/2} L_{\text{po}}^{3/2} / m_r^2 , \quad (7)$$

and the Maslov index is

$$\mu_{\text{po}} = 3m_r . \quad (8)$$

It follows from here that the partial periodic orbit sums A_n in eq. (4) should be calculated with order $n = m_r$. (The choice $n = \mu_{\text{po}} = 3m_r$ is also possible but the numerical calculations would be less robust because the order of the polynomials in the PA are increased by a factor of 3.) We included all periodic orbits with $m_r < 100$ in the PA to the function $g(k)$. The real and imaginary parts of $1/g(k)$ are presented as solid and dashed lines respectively in fig. 3. The zeroes of the function $1/g(k)$ agree perfectly to at least seven significant digits with the exact positions of the semiclassical eigenvalues obtained from eq. (5) and marked by the squares in fig. 3.

For chaotic systems the efficiency of semiclassical periodic orbit quantization can be estimated by comparing the length of the longest orbit included in the calculation with the Heisenberg period $L_H = 2\pi\bar{\rho}$ given by the average density of states. However, for integrable systems the nearest neighbour spacing statistics is a Poisson distribution with high probability of nearly degenerate levels. The lengths of periodic orbits should therefore be compared with the length $L_{\text{max}} = 2\pi/\Delta k_{\min}$ (with Δk_{\min} the smallest level spacing) rather than with the Heisenberg length. For the circle billiard, using orbits with period $L_{\text{po}} < 200$, it is no problem to resolve level spacings $\Delta k < 0.01$, *i.e.*, spacings where the characteristic length $L_{\text{max}} = 2\pi/\Delta k \approx 628$ is by more than a factor of three larger than the maximum length of the periodic orbits.

In conclusion, we have introduced the Padé approximant to perform summation of periodic orbit terms as a simple but powerful method for periodic orbit quantization. The Padé approximant allows the re-summation of the typically exponentially divergent terms of the semiclassical trace formulae. The method has been demonstrated on two systems with completely different classical dynamics, *viz.* the classically chaotic three-disk scattering problem and the integrable circle billiard. The Padé approximant can be applied when the total periodic orbit sum can be divided into partial sums with respect to an integer ordering parameter n . It is an interesting speculation if the latter might be related to the cycle length of periodic

orbits if a symbolic dynamics exists, or, in the general case, to the Maslov indices of orbits. Clearly, an in-depth investigation of this point will be worthwhile but goes beyond the scope of this Letter.

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